A SURVEY OF ENDF/B-VII(b1) COVARIANCE DATA AND RECOMMENDATIONS FOR MIGRATION TO ENDF/B-VII

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SUMMARY

A survey has been carried out of MF = 31, 32, 33, 35, and 40 covariance information taken from ENDF/B-VI.8 and included in ENDF/B-VII(b1) for consideration by CSEWG. No new covariance information has been submitted to ENDF/B-VII(b1) that was not already contained in ENDF/B-VI.8. Out of 386 individual materials contained in ENDF/B-VII(b1), there is covariance information of some sort or other provided for only 39 of these materials. However, for these materials covariance files were found for 371 specific MT numbers (since each material can include information for several MT process designations). A consequence from this review is that the individual covariance files for specific MT numbers associated with these materials were grouped into three quality categories : "good" (green), "marginal" (yellow), and "poor" (red) according to criteria defined in this report. The detailed results from this survey, including extensive comments on each entry, are included in an accompanying **EXCEL spreadsheet**. Following discussions with Pavel Oblozinsky and Michal Herman (NNDC), it was decided to recommend that only the covariance information judged to be worthy of belonging in the "good" category should be migrated to ENDF/B-VII (see the Appendix). The quantity of information recommended for migration is very limited (only 26 files), as is reflected in the following table:

MF	Quantity	Number of Materials	Number of Specific MT Covariance Files to Migrate
31	Nu-bar	4	2 out of 7 total
32	Resonance Parameters	4	1 out of 4 total
33	Cross Sections	36	21 out of 358 total [a]
35	Neutron Emission Spectra	1	1 out 1 total
40	Activation Cross Sections	1	1 out 1 total
	Totals	39 [b]	26 out of 371 total

[a] The numbers of specific MT covariance files available for materials where covariance information has been provided range from 1 to 17, with 10 individual MT covariance files per material being typical. Thus, the number of specific covariance files recommended for migration (only 21) is indeed a small fraction of the total number of available files.

[b] A few materials are represented in more than one MF category.

Covariance information from ENDF/B-VII(b1) perceived to be of lower quality, and therefore not recommended for migration to ENDF/B-VII, would not be lost to the user community if CSEWG accepts the present recommendations. Users could easily obtain this information by accessing ENDF/B-VI.8 if they so desire. This compromise approach establishes a relatively clean baseline for ENDF/B-VII without discarding potentially useful legacy information.

Introduction

A decision needs to be made by CSEWG by no later than June 2006 concerning the migration to ENDF/B-VII of covariance information from earlier evaluations included in ENDF/B-VI.8. The main tasks are to assess the quality of the existing information and to determine its utility to the users. The applied nuclear data user community is actively requesting covariance information because of a growing interest in assessing the safety, reliability, and cost uncertainties associated with modeling contemporary nuclear energy systems. The pursuit of these interests is facilitated by the ongoing development of sophisticated methods and software that enable the user community to perform such analyses. In order to proceed with this objective, covariance information must be available. In the near future, either the nuclear data evaluation community will provide this covariance information or users will be driven by necessity to generate their own uncertainty estimates.

The covariance information available in ENDF/B-VI.8 to carry over into ENDF/B-VII is quite limited. For example, there are evaluations for 387 materials in ENDF/B-VII(b1), but the number of these for which at least some covariance information has been provided is very limited: MF = 31 (4 materials); MF = 32 (4 materials); MF = 33 (36 materials); MF = 35 (1 material); MF = 40 (1 material). In order to provide a basis for deciding what, if any, covariance information should be migrated to ENDF/B-VII, it is essential to survey the information currently available. Due to the varied scope and quality of information available for specific materials, this is a task that involves the exercise of considerable subjective judgment in deciding what should be migrated. At one extreme is the approach that all the existing covariance information should be migrated. This is based on the argument that some information is better than none at all. At the other extreme is the idea that CSEWG should begin with a fresh start, and that the migration of existing covariance information, much of it of questionable quality, would tarnish the image of ENDF/B-VII as a superior product. In between these two extremes lies the possibility of selective migration of the best quality existing covariance information. This would represent a compromise solution to the problem facing CSEWG.

The present survey emphasizes the MF = 33 covariance data for smooth cross sections in the fast neutron region because most of the existing information that presently is available falls into this category. However, some additional comments are offered here concerning covariance information corresponding to the other listed MF categories.

Cross Section Covariances (MF = 33)

Criteria for assessing the quality of cross section covariances

Assessing the quality of existing covariance information is, by nature, a rather subjective undertaking owing to circumstances that are evident from the following discussion. Much of the existing covariance information was generated quite a few years ago (more than 20 in many instances) and thus needs to be judged in the context of those earlier times as well as in the framework of contemporary methods and requirements.

First, advances in computer hardware and software have been dramatic during the past 20 years. Few evaluators today can claim to be constrained in their activities by earlier computer-related limitations such as processor speed and storage capacity. However, this was not the case even as recently as ten years ago. Then, ENDF files were generally stored (and distributed) as tapes. Considerable effort (and cleverness) was devoted to avoiding redundancy in the content preserved on these tapes and to keeping the length of individual files at a minimum consistent with retention of the critical numerical information. Since covariance information can consume a lot of space (potentially something on the order of half the square of the number of evaluated data values), various ingenious space saving methodologies were developed by CSEWG evaluators that led to the development, acceptance, and utilization of a diversity of complicated formats for representing covariance information (e.g., refer to the ENDF formats manual, ENDF-102). It is evident from the present survey of the existing covariance files that widespread use has indeed been made of these various formats over the past two decades. One consequence of this state of affairs is that it is almost impossible to acquire a clear impression of the error magnitudes and correlations associated with the actual covariance matrices from an inspection of the information provided in the files without the aid of a covariance file processing code. This was a major handicap experienced by this reviewer in attempting to assess the quality of much of the available covariance information. As a consequence, it is the opinion of this reviewer that this state of affairs unnecessarily restricts the use of existing covariance matrix information to a select group of users who routinely have access to and use these processing codes, thereby limiting the potential "market" for covariance information to these "insiders". Also, it limits the possibilities for independent scrutiny of the quality and usefulness of covariance information in ENDF/B. In principle, it should not be necessary to rely on the use of sophisticated processing codes to carry out an independent review of the quality of evaluated cross section and covariance information, or to be able to visualize the uncertainties and correlations reflected by the recommended covariance matrices.

The first point this reviewer wishes to make is that these rather negative observations are not intended to serve as criticism of the steps taken by evaluators when these files were originally prepared. This reviewer recognizes that there were good reasons why earlier evaluators developed and used these formats. However, the need for continuing such arcane procedures no longer exists. ENDF/B files are no longer stored or distributed on "tapes". Storage capacity on transportable media (CD's, DVD's, memory sticks, etc.), as well as the ability to transmit large files over the Internet, insures that conservation of digital media "space" is no longer as critical an issue as it was in earlier times. It should now be quite feasible and appropriate to trade storage space for simplicity and transparency of the formats.

A second point this reviewer wishes to make is that the phenomenal growth of computing power has enabled sophisticated and more rigorous approaches to be introduced for generating covariance information rather than the former ad hoc methodologies. Comparisons between model-calculated results and available experimental data can be carried out on the fly through convenient and seamless access to the EXFOR database. This enables evaluators to make numerous fine adjustments to the parameter choices for the nuclear models used in the evaluations until acceptable agreement with data is obtained. Furthermore, this possibility, along with the growing body of documented information on parameter systematics, e.g., in the Reference Input Parameter Library (RIPL), enables evaluators to make reasonable estimates of the uncertainties in these model parameters. Finally, using both deterministic and Monte Carlo techniques, it is now quite feasible to propagate these model parameter uncertainties through to the computed observables such as cross sections, angular distributions, and particle emission spectra, and to merge these model-calculated results with experimental results in a seamless and statistically rigorous manner in order to generate optimal evaluations and corresponding covariance information. These newer, computationally intensive procedures yield complete covariance matrices for all included reaction channels, and even correlations between reaction channels if desired, in a consistent manner. Thus, for contemporary and future evaluations it no longer makes sense to generate covariance matrices based on ad hoc estimates of errors in the observables and such artifacts such as short-, medium-, and long range correlations. But, in all fairness, it must be stressed that these newer tools and computational capabilities were not available to evaluators when most of the currently available ENDF/B covariance information was generated. Only a very few reactions for a few materials included in this survey were evaluated using statistical methods that automatically generated covariance matrices.

These two points influenced this reviewer to make the following decision concerning the choice of criteria for rating existing covariance matrix information. The existing covariance information considered in the present review (included in an accompanying EXCEL document) has thus been classified according to the following three color-coded categories:

Good: These covariance entries are indicated by the color green. Good quality covariance entries are usually those that were produced by statistical analysis of experimental data and/or by explicit propagation of estimated model parameter uncertainties in a consistent way.

Marginal: The next category is marginally acceptable quality that is indicated by the color yellow. Those matrices that were generated from ad hoc evaluator estimates of uncertainties based on data errors and modeling limitations which, in most cases, were grouped into several distinct components intended to reflect estimates of short-, medium-, and long-range correlations for the constructed covariance matrices, fall into this category. Furthermore, to be included here the uncertainty estimates needed to encompass adequately detailed energy grids appropriate to the reaction processes in question. Those diagonal covariance matrices for reactions with high thresholds and (usually) relatively small cross sections, where the impact on neutronics calculations is generally modest, are sometimes also included in this category.

Poor: Poor quality entries are indicated by the color red. In this category are those covariance entries that were obviously generated using ad hoc uncertainty estimates on very crude energy grids, with no attempt made to provide any significant correlation information.

Other color codes are used to indicate reactions where no evaluations are present or where evaluations were made but no covariance information was produced. These codes are defined on an accompanying EXCEL spreadsheet. Furthermore, in some cases covariance matrices were generated for so-called “lumped” reaction processes. It is the opinion of this reviewer that such information may be of rather limited usefulness in applications because system-modeling computations, especially Monte Carlo simulations, frequently deal explicitly with specific physical reaction channels rather than hybrids. Consequently, it is not particularly useful to know that the sum of a particular collection of specific reactions has a particular uncertainty. Frankly, it is not clear to this reviewer how such information might be processed or handled in practical applications. Nevertheless, this reviewer understands how such “lumping” came about in various evaluations and sympathizes with the difficulty faced by evaluators in dealing with such situations. For example, one understandable reason that such a lumping approach might be pursued is that experimental data often are encountered in lumped form. In particular, neutron inelastic scattering to discrete but experimentally unresolved nuclear levels, or measurements of neutron-induced tritium production in light nuclei, where several distinct but experimentally indistinguishable physical processes are involved, can lead an evaluator to consider a lumping approach for a particular evaluation.

An attempt was also made in this survey to assign an overall quality “score” to the existing covariance information for each material considered within a particular MF category. The assigned score was either “good” (green), “marginal”(yellow), or “poor” (red) in much the same way as the ratings assigned to specific reactions, as described above. This summary score assignment for each material was based on two factors. The first was this reviewer’s assessment of the underlying quality of the covariance matrices available for the individual reaction channels considered for these materials. The second was the scope of the available covariance information for a particular material. In some cases the quality of individual covariance matrices was found to be reasonable but a lower overall score for the material was assigned simply because so few reaction channels were addressed by the original evaluator in generating covariance information. In fact, some of the covariance files for individual MT numbers with “good” scores have been recommended for migration even though the overall score for the material in question was lower. Once again, it must be stressed that these judgments are subjective, and they were made difficult by the proliferation of formats used for expressing covariance information as well as a lack of consistency from one material to the next and/or from one evaluator to the next. In large part, quality scores assigned here were influenced by this reviewer’s impressions concerning the amount of effort that appeared to have been expended by the individual evaluator in estimating uncertainties and the extent of the numerical detail which is provided in the file.

Results of the survey

As mentioned above, the results of the present survey of existing covariance information are presented in a companion EXCEL spreadsheet. Scores assigned to individual materials and reaction channels are evident at a glance as a consequence of the selected color scheme. Imbedded comments are included for all entries where covariance information was available. These comments provide details concerning the specific MF = 33 covariance entries contained in ENDF/B-VII(b1).

A quick glance at this spreadsheet shows that most of the entries carry the quality score “marginal” (yellow). This reviewer recognizes that the uncertainty information reflected in these files resulted, in most cases, from conscientious attempts on the part of the evaluators to convey their estimates of the uncertainties and correlations for their evaluated quantities using the tools available at the time that these evaluations were performed. Such estimates should not be dismissed lightly even though more sophisticated methods for generating covariance information are now available to evaluators. Original evaluators are the persons best qualified to assign errors to their evaluations, especially those based on subjective estimates of uncertainty. The final decision as to whether to migrate specific existing covariance information has to be made by CSEWG. However, it is the opinion of this reviewer, and one shared by Pavel Oblozinsky and Michal Herman, that only MF = 33 covariance information assigned the “good” score should be migrated. The reasons are given in the Appendix. Furthermore, it is recommended that other covariance information which did not qualify for the “good” score ought not to be discarded but should be accessible by users via ENDF/B-VI.8.

Some additional comments are in order concerning the cross-section covariance information available in ENDF/B. First, and foremost, it is surprising – shocking in fact – that so little MF = 33 covariance information is available for the heavy materials, and none is available for the actinides. Knowledge of cross section uncertainties for such important processes as neutron elastic and inelastic scattering, capture, and fission for key actinides such as U-235, U-238, and Pu-239, is essential for modeling studies of fission energy systems. Therefore, it should be a high-priority objective of the CSEWG community to generate this information for future Mod releases of ENDF/B-VII as soon as possible. The situation is somewhat more satisfactory for the structural materials but, for reasons discussed in the Appendix, only a few covariances files are being recommended for migration in this category. The situation for the lighter elements is, on the whole, quite unsatisfactory and should also be addressed by CSEWG in future Mod releases of ENDF/B-VII.

A vision for the future

During the process of carrying out the present survey of cross section covariance information, this reviewer could not resist the urge to envision and thus recommend improvements for the future. A goal for future evaluations should be to generate consistent covariance information for all physically allowed reactions for all materials included in ENDF/B, even if not all this information can be used initially for applications. The methodology for doing this exists and, if past history is a guide, user requirements will escalate steadily with the passage of time. Most modern reaction cross-section evaluations are generated using nuclear models so that they will be complete and physically consistent (partial reaction channels should add to the total cross section, etc.). Conscientious evaluators compare their modeling results with experimental data wherever these data are available. In cases where no data are available, the model calculations are frequently guided by systematics. Complete preliminary covariance matrices for all materials and reaction channels should be generated by propagating estimated parameter uncertainties for the parameters used in modeling. Either deterministic error propagation (based on sensitivity matrices) or Monte Carlo techniques could be applied in such analyses. These calculations should be performed only when the parameters have been fine-tuned to yield visual consistency with experimental data and conformance with systematics. The next step is to refine these matrices by actually merging the model calculated results (cross sections and uncertainties) with available experimental information by the method of generalized least squares. This Bayesian approach facilitates the combination of both objective (experimental) and subjective (modeling) results in a consistent way. The outcome will be smaller uncertainties in cases where extensive (and accurate) experimental data exist and larger uncertainties where only modeling is involved. Differences in the error correlations will also result from this merging process. By following this procedure, there will be uncertainty estimates generated for all materials and open reaction channels as well as covariances between reaction channels. Gaps in covariance information that are so commonly encountered with contemporary files need not exist in such a scheme. Applied users may not be able to utilize cross-reaction correlations at this time but, since the new evaluation methods will produce this information, at least some description of these correlations should be reported in the future by evaluators.

And now a few thoughts about formats for MF = 33 covariance information are presented. In the future, covariance matrices ought to be generated automatically by the same codes that are actually used to produce the evaluations themselves. There is a simple reason for this: a covariance matrix ought to correspond intimately to the procedures that are used for performing a specific evaluation as well as the data being evaluated. Covariance matrices provide quantitative measures of the uncertainty of the evaluation procedure as well as of the underlying objective and subjective information incorporated in the analysis. So, there is no such thing as a universally "correct" covariance matrix. From a practical point view, automatic generation of the covariance matrix is a great labor saving step, and this approach also avoids introduction of numerical errors as is more likely to happen when ad hoc methods are used. Two modern evaluation codes, TALYS and EMPIRE, currently offer options for outputting evaluation results in ENDF format. Extensions to also produce covariance information in an appropriate ENDF format should be the next development step, and this is currently being worked on within the nuclear data community. In this scheme, most of the complex formats used for representing cross-section covariance matrices (MF = 33) that have been used in the past should be avoided. Cross-section covariance information should be represented in the files by explicit relative covariance matrices (fractional errors and correlations). This information should appear in an ENDF covariance file as single a component (NI-type, LB = 5) with no add-ons such as the LB = 8 component that was frequently included in the past to avoid singularities that might be introduced during file processing (see below). This format represents explicit covariance information in terms of fractional errors and correlations rather than absolute variances and covariances. Relative covariance matrices have the desirable feature that they normally do not have to be altered when a few minor adjustments are made to the evaluated cross sections themselves. If desired, these matrices could be generated on a somewhat coarser grid than the actual evaluations themselves to conserve space, but they should always be generated directly from applications of the evaluation codes using the same input information. For example, one might wish to represent a total cross section in the fast neutron energy range for a structural material with 1000 energy grid points but use only 20 to 50 energy grid points to represent its covariance matrix adequately. This could be accomplished easily by performing the same evaluation twice with the two different energy grids, but always using the same model parameters and experimental data in these analyses. This approach applies equally well to those matrices that correspond to physical quantities that are derived indirectly from other information. For example, the Monte Carlo approach to propagating uncertainties can automatically handle error propagation for derived quantities that are based on sums and/or differences of other quantities just as well as it can individual reaction channels. All these procedures should be practical as well as feasible using contemporary computers and the modern evaluation computational tools that are currently available or under development.

By settling on a single format for cross section covariance information in the fast-neutron region one could realize a number of useful simplifications. The evaluation code output routines could be simpler and file checking and validation codes would be easier to maintain since they would not have to deal with as many different formats as is currently the case. Also, convenient on-line utility programs could be implemented at the nuclear data centers for explicitly listing the uncertainties (from the diagonal elements of the matrices) or plotting them as error bands, along with the evaluations and existing experimental data, for useful visualization. Correlation matrices could be plotted in two dimensions or as 3-D perspective images using such routines, again in order to aid in their visualization. Having such utility routines readily available would make it much easier for independent reviewers to judge the quality of the available covariance information and for users to gain a feel for the uncertainties associated with individual evaluations.

This reviewer is not suggesting that the existing format structure developed for ENDF/B covariance information needs to be discarded entirely and replaced, but rather it is suggested that most of the formats that have been used in the past should be "retired" from active duty (i.e., marginalized) in the new evaluation scheme, except in situations when they are absolutely needed. Furthermore, evaluators ought to be discouraged from using unneeded formats in the future. This includes the "infamous" LB = 8 format mentioned briefly above that has been used in add-on covariance components with the intent to avoid singularities in matrices that sometimes develop when covariance information is processed into arbitrary (usually finer) group structures by processing codes. Singularities that may originate through file processing have no significant impact when covariance matrices are used for uncertainty propagation. Mathematical problems are encountered only when such matrices need to be inverted, e.g., in data adjustment or data merging exercises. It is the recommended by this reviewer that matrix singularity should be automatically tested in user codes and, where necessary, small ad hoc and insignificant additions could be applied automatically to the variances (diagonal elements) to remedy the problem of singularity without introducing any significant negative effects. In other words, the consequences of manipulating the covariance information contained in ENDF/B files through processing into arbitrary group structures or other user-defined formats should be borne by the user community and not CSEWG or the ENDF evaluators.

Other Covariances (MF = 31, 32, 35, and 40)

The other covariance information available in ENDF/B-VII(b1) is quite limited. It consists of uncertainty information for nu-bar (MF = 31), low-energy resonance parameters (MF = 32), energy distributions of secondary emitted particles (MF = 35), and production of radioactive nuclei (MF = 40). Comments and judgments regarding this information appear on separate sheets of an accompanying EXCEL document mentioned above.

This reviewer is not well acquainted with the resonance region, so the quality judgments and general comments expressed here are based largely on subjective perceptions of the amount of effort apparently expended by the evaluator and the numerical detail provided, as reflected in the individual numerical values and file documentation. The procedures used to evaluate cross sections for the thermal region, the resonance region, the unresolved resonance region, and the fast-neutron region are quite distinct and likely will remain so for the foreseeable future. As a consequence, there are really few if any uncertainty correlations between these regions (unless one includes the potential longer-range effects of broad resonances that may introduce some correlations between these regions for certain materials). The generation of reasonable covariance information for the resonance region, and its representation in practical terms, is an issue that will need to be addressed by CSEWG experts in the years ahead. The objective should be to simplify the procedures currently used and to make the information more readily available and transparent for visualization and review purposes while at the same time assuring adequacy for a broad range of user applications. It is well known that users tend to energy average the information in this region by introducing group structures, sometimes just a few groups to span the entire resonance region. One then has to wonder just how useful complete detail on the individual resonance parameter uncertainties could possibly be under these circumstances. Also, the uncertainty information for this region is normally processed by users into a form resembling MF = 33 cross section covariances. One can speculate that perhaps many users would be satisfied with actual cross section covariance information from ENDF/B rather than detailed covariances for the resonance parameters from which these cross sections are computed. If so, then this would suggest bypassing the need for using MF = 32 formats in the future. Of course, in principle one could argue that it is possible to propagate resonance parameter uncertainties and thereby estimate their effects on the derived cross sections or other physical quantities. But, for the heavier materials, such as the actinides, this can become an almost prohibitive computational challenge, even with modern computers, since thousands of resonances are involved. Why bother doing this if most of the detailed information that might be provided in MF = 32 formats is eventually averaged out by the file processing procedures invoked by users? In any event, issues and problems concerning the reporting and handling of covariance information for the resonance region should not impede the generation of covariances for the unresolved resonance and fast-neutron energy regions where the situation is more straightforward.

The covariance information for nu-bar (prompt, delayed, and total) is presented in considerable detail for the four materials covered. The quality of covariance information for U-235 appears to be the best of the lot in that it was generated for the most part from a detailed quantitative analysis of experimental information. It is recommended for migration to ENDF/B-VII in spite of some reservations concerning the formats (see the Appendix). However, the information for the other three materials may be adequate since in those cases the uncertainty information, though largely based on ad hoc evaluator estimates, has nevertheless been guided by consideration of compiled experimental data. This information is not recommended for migration but can always be obtained from ENDF/B-VI.8.

The only MF = 35 neutron-emission spectrum covariance information available is that for Cf-252 spontaneous fission, and that is of excellent quality owing to the considerable effort expended in making this a standard and carefully estimating the corresponding uncertainties. This covariance file is recommended for migration to ENDF/B-VII with no anticipated issues related to format issues.

Finally, the evaluation as well as the MF = 40 covariance information for production of Nb-93m by neutron inelastic scattering on mono-isotopic niobium is based on a statistical analysis of experimental data and nuclear modeling results. It should be considered as having good quality, and this covariance file is recommended for migration to ENDF/B-VII with no anticipated problems related to format issues.

Appendix

Recommendations to CSEWG

A decision needs to be made by CSEWG by no later than June 2006 concerning the migration of covariance information presently contained in ENDF/B-VII(b1) to ENDF/B-VII. To aid in this decision, specific recommendations are given below based on the results of the present review and discussions held by the reviewer with Pavel Oblozinsky and Michal Herman during a 23-27 January 2006 visit to BNL. The quantity of covariance information recommended for migration as a consequence of this exercise is quite limited, as is clearly evident from the following table (which also appears in the Summary):

MF	Quantity	Number of Materials	Number of Specific MT Covariance Files to Migrate
31	Nu-bar	4	2 out of 7 total
32	Resonance Parameters	4	1 out of 4 total
33	Cross Sections	36	21 out of 358 total [a]
35	Neutron Emission Spectra	1	1 out 1 total
40	Activation Cross Sections	1	1 out 1 total
	Totals	39 [b]	26 out of 371 total

[a] The numbers of specific MT covariance files available for materials where covariance information has been provided range from 1 to 17, with 10 individual MT covariance files per material being typical. Thus, the number of specific covariance files recommended for migration (only 23) is indeed a small fraction of the total number of available files.

[b] A few materials are represented in more than one MF category.

However, since all of the covariance information contained in ENDF/B-VII(b1) was obtained from ENDF/B-VI.8, that legacy covariance information which is not recommended for migration to ENDF/B-VII will be readily available to interested users via access to ENDF/B-VI.8. Therefore, there should be no grounds for concern that it will be lost to the nuclear science community if migration should indeed be limited to only the recommended covariance files.

Nu-bar (Neutrons per Fission) Covariances

Recommendations - File 31 Covariances Migration

Based on a survey conducted by D.L. Smith (Argonne) and discussions held during 1/23-27/2006 at the NNDC

Key:
None (Migrate no covariances)
Yes: a,b,c, … (Migrate MT = a,b,c, …covariances)

Element	Isotope	Recommendation	Comments
Uranium	U-235	Yes: 452,456	ENDF/B-VI MOD 2 Revision 1; D. Hetrick (1980); T.R. England (1989)
	U-238	None	

Plutonium	Pu-240	None
	Pu-241	None

Discussion:

It is recommended to migrate the indicated covariance information to ENDF/B-VII because of the considerable importance of nu-bar for applied fission technology. The quality of existing covariance information for U-235 is considered to be good above and beyond the issue of formats. However, the question of formats should be addressed in the future, as discussed above. Since this reviewer is not very familiar with File 31 formats currently adopted by CSEWG and documented in ENDF-102, it is not appropriate to comment on them or to offer constructive suggestions related to future format policy. However, it is strongly recommended here that CSEWG give consideration to this matter in planning for future releases of ENDF/B.

Resonance Parameter Covariances

Recommendations - File 32 Covariances Migration

Based on a survey conducted by D.L. Smith (Argonne) and discussions held during 1/23-27/2006 at the NNDC

Key:
None (Migrate no covariances)
Yes: a,b,c, … (Migrate MT = a,b,c, …covariances)

Element	Isotope	Recommendation	Comments
Sodium	Na-23	Yes: 151	ENDF/B-V; D.C. Larson (1977)
Plutonium	Pu-240	None	
	Pu-242	None	
	Am-241	None	

Discussion:

It is recommended to migrate the indicated resonance parameter covariance information to ENDF/B-VII because of its considerable importance for applied technology. The quality of covariance information is considered to be good. However, this reviewer would prefer to see this covariance information presented in terms of cross section rather than resonance parameter uncertainties in a recommended File 33 format rather than in terms of File 32 formats. The broad question of formats for resonance covariance information needs to be addressed in the future, as discussed above. Since this reviewer is not familiar with File 32 formats currently adopted by CSEWG, documented in ENDF-102, and used by evaluators, it is not appropriate to comment on them or to offer constructive suggestions for format policy in the future beyond the speculations mentioned above concerning the matter of how this information is actually handled by applied users. However, it is strongly recommended that CSEWG give consideration to this matter in planning for future releases of ENDF/B.

Cross Section Covariances

Recommendations - File 33 Covariances Migration

Based on a survey conducted by D.L. Smith (Argonne) and discussions held during 1/23-27/2006 at the NNDC

Key:
None (Migrate no covariances)
Yes: a,b,c, … (Migrate MT = a,b,c, …covariances)

Element	Isotope	Recommendation [a]	Comments
Lithium	3-Li-7	Yes: 1	ENDF/B-V.2; P.G. Young (1981)
Carbon	6-C-0	None	
Fluorine	9-F-19	Yes: 4,16,22,28	ENDF/B-VI.1; Z.X. Zhao, C.Y. Fu, D.C. Larson (1990)
Sodium	11-Na-23	None	
Silicon	14-Si-28	None	
	14-Si-29	None	
	14-Si-30	None	
Titanium	22-Ti-48	Yes: 1,4,16,28,102,103,107	JENDL 3.3; T. Asami (1988,2003)
Vanadium	23-V-0	Yes: 1	ENDF/B-VI.1; D.L. Smith (1988)
Chromium	24-Cr-50	None	
	24-Cr-52	None	
	24-Cr-53	None	
	24-Cr-54	None	
Manganese	25-Mn-55	None	
Iron	26-Fe-54	None	
	26-Fe-56	None	
	26-Fe-57	None	
	26-Fe-58	None	
Cobalt	27-Co-59	Yes: 1,16,103,107	ENDF/B-VI.1; D.L. Smith (1989)
Nickel	28-Ni-58	Yes: 16	ENDF/B-VI.1; A. Pavlik and G. Winkler (1983)
	28-Ni-60	None	
	28-Ni-61	None	
	28-Ni-62	None	
	28-Ni-64	None	
Copper	29-Cu-63	None	
	29-Cu-65	None	
Niobium	41-Nb-93	Yes: 1	ENDF/B-VI.1; D.L. Smith (1985)
Rhenium	75-Re-185	None	
	75-Re-187	None	
Gold	79-Au-197	Yes: 1	ENDF/B-VI.1; P.G. Young (1984)
Lead	82-Pb-208	None	
Bismuth	83-Bi-209	Yes: 1	ENDF/B-VI.1; D.L. Smith (1989)
Uranium	92-U-238	None	
Plutonium	94-Pu-240	None	

	94-Pu-242	None
Americium	95-Am-241	None

[a] Migrate only a relative covariance matrix (NI-type, LB = 5) obtained from statistical analysis and/or model parameter error propagation. Eliminate any LB = 8 components that may have been added afterwards and included in ENDF/B-VI.8 covariance files.

Structures of the "Good" Category Covariance Files

			Covariance Components [a]			
Isotope	MT	Method [b]	LB=1	LB=5	LB=8	Other [c]
Li-7	1	S		1		1
F-19	4	P	1	4	1	
	16	P		3	1	
	22	P		2	1	
	28	P		1	1	
Ti-48	1	S		1		
	4	S		1		
	16	S		1		
	28	S		1		
	102	S		1		
	103	S		1		
	107	S		1		
V-0	1	S		1		
Ni-58	16	S		1	1	
Co-59	1	S		1		
	16	S		1		
	103	S		1		
	107	S		1		
Nb-93	1	S		1		
Au-197	1	S		1		
Bi-209	1	S		1		

[a] Actual covariance matrix is constructed from indicated components.
[b] Method of derivation of the covariances: S = statistical analysis of data; P = parameter uncertainty propagation.
[c] Other File 33 covariance component formats adopted by CSEWG.

Discussion:

Following extensive discussions with Pavel Oblozinsky and Michal Herman, it was decided to recommend that only those 21 MF = 33 cross-section covariance files that were assigned the "good" score in an accompanying EXCEL document, as indicated in the two preceding tables, should be migrated to ENDF/B-VII. Ideally, this information ought to have originated from a rigorous statistical analysis of experimental data and/or propagation of nuclear model parameter uncertainties in a consistent manner. The covariance file should also be stand-alone. That is it should not refer to information for any other material or MT number. Finally, this covariance information should be presented as a single, explicit relative covariance matrix

(NI-type, LB = 5). All the 21 MT = 33 covariance files proposed for migration are considered to be of "good" quality and were generated from either a statistical analysis or model parameter uncertainty propagation. However, only 15 of these files satisfy the rigid format criteria exactly. Two additional files would satisfy the format requirements if the LB = 8 components were dropped. It might be possible to convert those files where one or more formats other than LB = 5 were used to a single LB = 5 file, but this would most likely require running a processing code. By recommending that migration of existing covariance files be restricted to those with formats which are fairly consistent with the objective of simplicity in the majority of cases, it is hoped that the first release of ENDF/B-VII covariance files will reflect a relatively "clean slate" upon which to build in the future. It will then be proposed to CSEWG that strong restrictions be placed on the use of the current suite of adopted File 33 formats in future new or updated evaluations that will be included in Mod releases of ENDF/B-VII or beyond.

Applying these rather stringent constraints for migration of File 33 information to ENDF/B-VII resulted in a relatively small list of recommended MF = 33 covariance files to be migrated. This reviewer recognizes, and Pavel Oblozinsky and Michal Herman agree, that much of the earlier covariance information originally from ENDF/B-VI.8, and carried over to ENDF/B-VII(b1), might be reasonably reliable and therefore potentially useful for some applications. Consequently, it should not be lost. Thus, it is proposed that users be referred to ENDF/B-VI.8 for this non-migrated material. Steps will be taken to insure that ENDF/B-VI.8 can be obtained readily from the data centers.

Neutron Emission Spectrum Covariances

Recommendations - File 35 Covariances Migration

Based on a survey conducted by D.L. Smith (Argonne) and
discussions held during 1/23-27/2006 at the NNDC

Key:
None (Migrate no covariances)
Yes: a,b,c, … (Migrate MT = a,b,c, …covariances)

Element	Isotope	Recommendation	Comments
Californium	Cf-252	Yes: 18	ENDF/B-VI.1; W. Mannhart (1989)

Discussion:

It is recommended to migrate this covariance information for neutron emission spectra to ENDF/B-VII because of its considerable importance for applied technology. The quality of covariance information is considered to be excellent. Since this reviewer is not familiar with File 35 formats currently adopted by CSEWG and documented in ENDF-102, it is not appropriate to comment on them or to offer constructive suggestions for format policy in the future. However, it is strongly recommended that CSEWG give consideration to this matter in planning for future releases of ENDF/B.

Activation Cross Section Covariances

Recommendations - File 40 Covariances Migration

Based on a survey conducted by D.L. Smith (Argonne) and
discussions held during 1/23-27/2006 at the NNDC

Key:
None (Migrate no covariances)
Yes: a,b,c, … (Migrate MT = a,b,c, …covariances)

Element	Isotope	Recommendation	Comments
Niobium	Nb-93	Yes: 4	ENDF/B-VI.1; D.L.Smith and L.P. Geraldo (1990)

Discussion:

It is recommended to migrate this information to ENDF/B-VII because of its considerable importance for applied technology. The quality of covariance information is considered to be good. The format used is essentially that recommended for File 33 (NI-type, LB = 5).

Attachment

EXCEL spreadsheet is given separately. It contains detailed comments on File 31, File 32, File 33, File 35 and File 40.